- *Low Separation Rank Approximations for Application of the Square Root of Laplacian in 3-D* by Gregory Beylkin and Fernando Perez, University of Colorado at Boulder, George I. Fann, Oak Ridge National Laboratory (fann_laplacian_2006.pdf)

  We've derived and developed a new fast O(N) method for computing and applying the inverse square root of the Lapacian operator in 3D based on adaptive, multiresolution low-separation- rank representations of functions and operators. These multiwavelet representations are being applied to computational chemistry and material simulations and are accurate up to arbitrary but finite precision.

- *Evaluation of Supersingular Integrals: Second Order Boundary Derivatives* by Matthew N. J. Moore, L. J. Gray and T. Kaplan
  Oak Ridge National Laboratory (gray_supersingular_2006.pdf)

  A standard boundary integral equation solution of a partial differential equation results in knowledge of the principal function and its normal derivative everywhere on the boundary. This work has established that all second order boundary derivatives of this function can also be computed, even with a boundary interpolation that is simply continuous between elements. This higher order derivative information is expected to be useful for problems that require a nonlinear solution iteration, e.g. contact analysis, topology optimization, etc.

- *Large Scale Simulation of Fracture in Disordered Materials* by Phani K. Nukala and Srdjan Simunovic, Oak Ridge National Laboratory (nukala_RFM_2006.pdf)

  Computational modeling of fracture in disordered materials using discrete lattice models is limited to small system sizes due to high computational cost associated with re-solving the governing system of equations every time a new lattice bond is broken. We proposed an efficient algorithm based on multiple-rank sparse Cholesky downdating scheme for 2D simulations, and an iterative scheme using block-circulant preconditioners for 3D simulations. Based on these algorithms, we were able to simulate largest ever 2D (e.g., L = 1024) and 3D lattice systems (e.g., L = 64) that advanced our understanding over many controversial issues. Still larger system sizes are required in 3D to obtain fundamental understanding of scaling laws and size-effect of fracture, and we have recently simulated fracture of a 128^3 system in 3D using 512 processors of IBM Blue Gene/L.

- *A Coarse Graining Procedure For Including Correlation Beyond Mean-Field Theory:" A Multiscale Method That Goes Beyond Traditional Homogenization"* by W.A. Shelton, Oak Ridge National Laboratory, D. Biava and D.D. Johnson, University of Illinois (Champaign) (shelton_NLCPA_2006.pdf)

  We have developed a fully 3D nonlocal coherent potential approximation (NLCPA) method for treating the effects of substitutional disorder on the electronic structure and total energy that goes beyond traditional mean-field theories by including additional short-range correlation. The method systematically provides a hierarchy of improvements on the traditional mean-field theory based coherent potential approximation that is used to self-consistently treat the effects of substitutional disorder on the electronic structure. The

NLCPA has a rather broad applicability to various scientific domains including materials science, chemistry, solid-state physics, etc. In particular, this approach when combined with electronic structure methods can be used to treat systems where charge correlation, spin fluctuations and lattice displacement effects are important.

- *Fast Green's Function Updates in Dynamic Cluster Approximation* by E. F. D'Azevedo and T. Maier, Oak Ridge National Laboratory (dazevedo_green_2006.pdf)

  Dynamic Cluster Analysis with Quantum Monte Carlo is used to model high-temperature superconductivity in highly correlated electronic systems. The main computational kernel is a rank-one update of the Green's function matrix. This operation is sensitive to memory bandwidth and achieves only a small fraction of peak performance on most scalar processors. A new algorithm delays the updates to be performed as a more efficient matrix-matrix multiply operation. This achieves nearly a five-fold speedup on most processors.

- *Householder Fellowship* by Richard Archibald, Oak Ridge National Laboratory (archibald_edge_2006.pdf)

  The Alston S. Householder Fellowship provides new computational scientists with opportunities to pursue research in pure and applied mathematics in an area related to high-performance scientific computing and in a scientific area aligned to the missions of the Department of Energy. Generalized boundary and singularity detection with specific application to post-processing techniques for discontinuous Galerkin (DG) methods for linear hyperbolic equations have been developed under funding from this Fellowship.

- *Green's Function Evaluation for Three-Dimensional Exponentially Graded Elasticity* by L. J. Gray, Oak Ridge National Laboratory, R. Criado, V. Mantic, F. Paris, University of Seville, Spain (gray_fgm_2006.pdf)

  The ability to numerically model the behavior of Functionally Graded Materials (FGMs) is key to their development and optimization for specific engineering applications. In this project, the expressions for the fundamental solution (Green's function) for a three-dimensional exponentially graded material have been implemented. With the ability to compute the Green's function, FGM problems can be solved by means of a boundary integral equation formulation. By solving problems having known exact solutions it has been demonstrated that the complicated expressions for the fundamental solution, and their numerical evaluation, are correct.

- *Fast Solution of 3D Boundary Integral Equations by a Precorrected-FFT* by S. Nintcheu Fata, L. J. Gray, and T. Kaplan, Oak Ridge National Laboratory (gray_pfft_2006.pdf)

  A new Fast Fourier Transform-based algorithm (Precorrected-FFT [PFFT]) to rapidly solve boundary integral equations has been developed. This new technique employs a regular grid and FFT to quickly evaluate boundary integrals in a sparse manner. The sparse representation of the coefficient matrices results in a significant reduction in the memory requirements and computational time. The PFFT can therefore be used to solve problems involving large-scale simulations with complicated geometry.

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